Influence of agglutination on appearance of ink on white paper.

K. Bartkiewicz[1)], S.V. Ershov[2)], S. G. Pozdnyakov[3)], A.G. Voloboy[2)], K. Tsuchiya[4)], N. Kirilov[4)]

Faculty of Physics, Adam Mickiewicz University (Poland)[1)],
KIAM, Russian Academy of Sciences (Russia) [2)],
Moscow Engineering Physics Institute (Russia)[3)]
Integra Inc. (Japan)[4)]

E-mail: *voloboy@gin.keldysh.ru*

We investigate influence of agglutination of pigment particles on appearance of ink printed on white paper. Agglutination patterns are created by simulating thermal motion of pigment particles and inter-particle interaction. The appearance of the ink layer on white paper is calculated in framework of scalar diffraction theory by Integra software. The software provides integrated visual computing environment for analysis of light scattering in advanced coatings (filters, ink, paint, cosmetics etc).

1 Introduction

A physically accurate simulation of optical properties of *inks* happens to be a not trivial problem and the simple absorption laws like Beer's are insufficient. This is because ink is not an ideally homogeneous substance but a suspension of some, yet small, pigment particles in a "binder". In spite being small as compared to pigments used in paints[1),2)], they are not as tiny as to neglect their size treating the ink medium as homogeneous. To calculate light reflection and transmission in an ink layer, one must solve diffraction problem with those particles[1)]. And here the *agglutination* effect is of extreme importance. Indeed, very small ink particles scatter light rather weakly, but when (or if) they glue in large "cluster", they behave like "effective particles" of much larger size and thus different light scattering properties. So our work consisted of two parts: (1) calculation of the distribution of particles in simulation domain with and without agglutination (2) calculation of light diffraction in that geometry.

A physically correct simulation of the agglutination process is an extremely complex problem of a highly viscous hydrodynamics at molecular level, with molecular-level chemical based affinity forces, which includes many physical and chemical parameters e.g. Hamaker constant[3)] which are not always known.

In our work we present agglutination patterns obtained by applying a simple model of agglutination process based on an idealized Brownian motion and particle interaction which requires very small number of usually available physical parameters as, e.g., viscosity of ink or gravity of pigment material[3)]. Despite the model being highly idealized it provides ink layer geometry instances similar to the ones reported in literature [3)].

2 Principle

Preparation of geometry of an ink layer for optical simulation is performed in two stages. First, we create a statistically uniform 3D spatial distribution of pigment particles. Later, we simulate random thermal motion of *adhesive* particles i.e. they glue to each other (with some probability) when and only when they hit each other and do not attract at distance. This is a good approximation for affinity forces (like hydrophilic-hydrophobic) in a highly viscous material. The motion of the particles or clusters in our model is Brownian under stochastic delta-correlated force. As yet we neglected rotational diffusion. These equations of motion are integrated numerically until the expected agglutination level is achieved. The resulting geometry is used in scalar wave optical simulation.

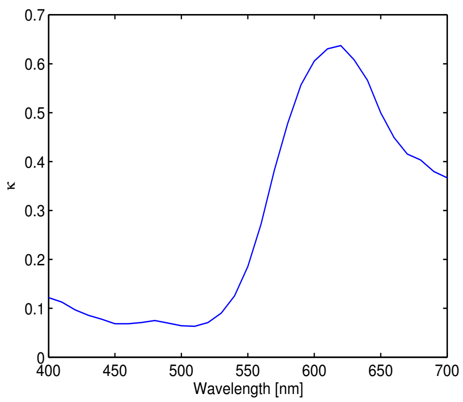

Fig.1 Imaginary part of refractive index for blue pigment.

Optical simulation of printed ink with a complete vector description of light is computationally expensive and for stochastic structures, like printed ink, has little advantage over scalar diffraction theory[2)]. In our work we apply scalar wave theory based Ink Simulator (Integra Inc.). The Ink Simulator solves a scalar diffraction problem in frequency domain for an arbitrary ink layer[2)]. Moreover, it post processes the obtained results to account for an arbitrary paper substrate. The output of the program consists of BRDF (Bidirectional Reflectance Distribution Function) file of ink layer on paper and of visualization of the BRDF. For appearance simulation we use a blue pigment material of real part of refractive index equal to 1.4 and imaginary part of refractive index as shown in Fig.1.

3 Experiment

The model of agglutination is highly idealized, however but in case of various colloids a similar aggregation mechanism turned out to be universal[4]. This appears to be confirmed by visual investigation of generated agglutination patterns against the real compositions (see Fig.2. TEM image reprinted with permission from Ref.[3]. Copyright 2010 American Chemical Society.)

We generated of agglutination patterns for blue pigment material (other than CuPc) representing three levels of the agglutination and simulated appearance of the composition with Ink Simulator. For the simulations we used particle volumetric concentration PVC = 15%, simulation domains of size 5.12 x 5.12 x 0.5 μm, and a white plane parallel illumination. The result is appearance of the printed ink on white paper (see Fig.3 and Fig.4).

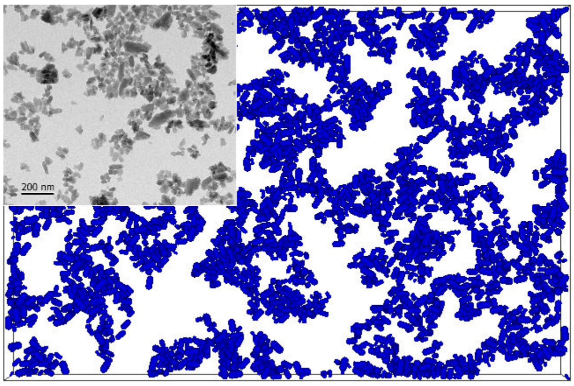

Fig.2 Superimposed TEM image of CuPc pigment particles[3] over corresponding computer generated geometry.

4 Conclusion

We demonstrate that computer simulation of agglutination and light scattering on ink printed on white paper is possible. Our results agree with experimental observations. Our generated geometry corresponds to real one. The elaborated software provides integrated visual computing environment ensuring analysis of light propagation in optically complex materials with light scattering in stochastic geometries common to all kind of advanced coatings including filters, ink, paint, cosmetics, etc, necessitating the use wave optics laws.

We demonstrate that agglutination influences the final appearance of printed ink. Agglutination also affects flip-flop (iridescence) phenomenon that occurs for thin coating layer. The stronger agglutination, the stronger is the flip-flop effect of the resulting color (see Fig.3 and Fig.4).

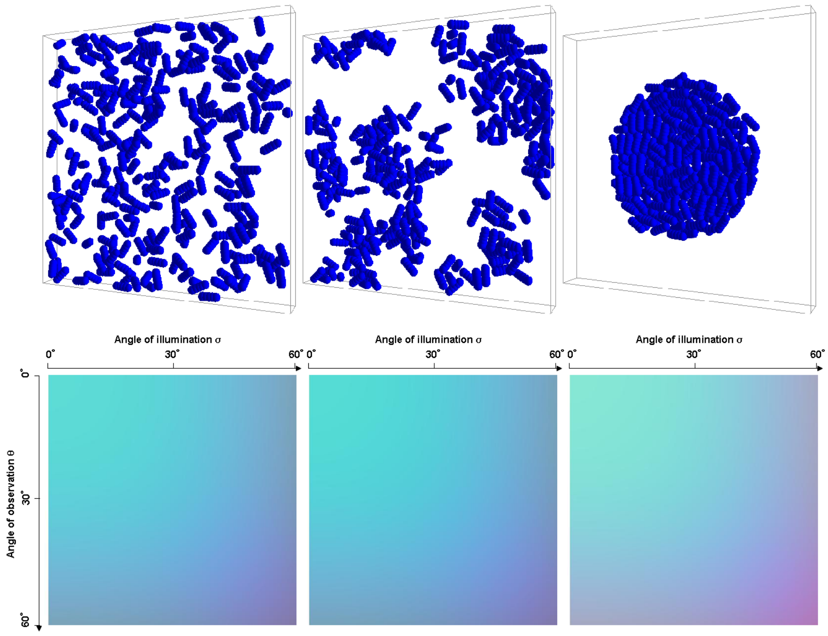

Fig.3 Influence of agglutination of blue pigment on appearance of ink. From left: (a) no agglutination, (b) agglutination (mean cluster size 10% of particles), (c) deterministic case – single cluster.

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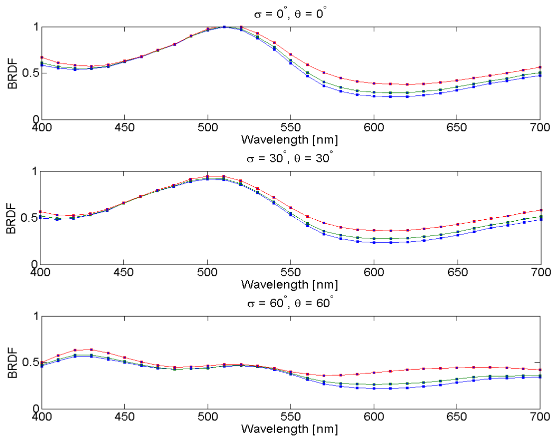

Fig.4 BRDF: blue, green, and red curves correspond to cases (a), (b), and (c) from Fig. 3, respectively.

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